

Safety Guide 100

**DESIGN GUIDE FOR PACKAGING AND OFFSITE TRANSPORTATION
OF NUCLEAR COMPONENTS, SPECIAL ASSEMBLIES, AND RADIOACTIVE
MATERIALS ASSOCIATED WITH THE NUCLEAR EXPLOSIVES
AND WEAPONS SAFETY PROGRAM**

CHAPTER 6.0

CRITICALITY ASPECTS

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ACRONYMS

AEG	Average Energy Group
ANSI	American National Standards Institute
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
CFR	Code of Federal Regulations
CI	Criticality Index
DOE	Department of Energy
DOT	Department of Transportation
HAC	Hypothetical Accident Conditions
HEU	Highly Enriched Uranium
LEU	Low-Enriched Uranium
NCT	Normal Conditions of Transport
NRC	Nuclear Regulatory Commission
RI	Radiation Index
SARP	Safety Analysis Report for Packaging
TI	Transport Index

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6.0 CRITICALITY ASPECTS

6.1 INTRODUCTION

6.1.1 Scope

This chapter of the design guide has been prepared as an aid to the nuclear criticality safety analyst in the design phase of the package development and in performing and documenting the nuclear criticality safety evaluation (usually Chap. 6) of the Safety Analysis Report for Packaging (SARP).

6.1.2 Approach

The approach developed in this chapter is first to address the design issues that the criticality safety analyst might identify as being primary design requirements. The second is to address design issues that will enhance criticality safety (specifically subcriticality) but that are not primary criticality safety design requirements. These issues and concepts are addressed in the following section.

Section 6.2 reviews the regulatory requirements from the perspective of nuclear criticality safety. Sections 6.3 through 6.8 provide guidance for performing and documenting the evaluation for package approval and certification.

6.1.3 Design Process

6.1.3.1 Determination of need for watertightness

The principal impact that nuclear criticality safety has on a package design is the necessity for watertightness, which is dependent primarily upon the contents to be shipped. Regulations (to be discussed in more detail later) require that a package used for the shipment of fissile material be so designed and constructed and its contents so limited that it would be subcritical if water were to leak into the containment system so that maximum reactivity would be attained with the containment system closely reflected by water on all sides. This regulation is imposed without regard as to how or when the water leakage occurs, the conditions of transport, or whether the packaging has been damaged. The assessment of maximum reactivity should be consistent with the chemical and physical form of the material and the credible extent to which moderation can occur.

Herein lies the basic criticality safety input requirement to the package design. With the proposed loading and a conceptual design of the containment system (i.e., inner container dimensions and volume), the criticality safety analyst must first determine if the contents remain adequately subcritical if water inleakage were to occur (to the most reactive and most credible extent).

If the proposed contents in a single package are adequately subcritical for the assumed water leakage conditions, the impact of criticality safety requirements on the design will probably be negligible. However, if the proposed contents in a single package (for the assumed conditions) are not adequately subcritical, the following three options are available: 1) is to reduce the contents quantity and/or reduce the dimensions of the containment system, 2) is to add neutron poisons to the fissile material, or 3) is to pursue an exception to the water-inleakage requirement.

Option 1, reducing the contents quantity and/or reducing the dimensions of the containment system, may be feasible if the package is being designed to transport bulk or loose materials (e.g., metal pieces, powders, small parts, etc.). However, this option will not be available if the contents are large parts or weapon components for which the mass and dimensions are fixed.

Option 2, adding a neutron poison to the fissile material, may be feasible for bulk or loose materials if the neutron poison material can be properly intermixed or placed in the fissile material. However, this option may present unacceptable operational control problems (e.g., ensuring that the poison material is always present and in the quantity and position required by criticality safety). Use of this option is common in the transport of commercial power reactor fuel assemblies but is generally not practical for the transport of other types and forms of fissile material.

Option 3, obtaining an exception from the water leakage requirements, is frequently the only option available for large parts and weapon components. This option takes credit for any leak tightness incorporated into the package design, but it also requires additional package design features and special requirements that would not otherwise be needed.

6.1.3.2 Exception to the water-inleakage requirement

As discussed in the preceding section, a package used to transport fissile material must be subcritical if it is assumed that water were to leak into the containment system so that maximum reactivity is attained with the containment system closely reflected by water on all sides. An exception to the water in-leakage requirement may be approved by the certifying authority if the package design incorporates special features that ensure that no single packaging error would permit leakage and if appropriate measures are taken before each shipment to ensure that the containment system does not leak. The

adequacy of both the special design features and the appropriate measures before each shipment has, in the past, been a source of considerable controversy.

The following are generally considered necessary to satisfy these two requirements:

1. Special features - should include multiple containment boundaries, each meeting the minimum leak rate criteria (e.g., watertightness), each containment boundary is leak rate testable, and each containment boundary remain watertight after being subjected to the hypothetical accident conditions tests, and
2. Appropriate measures before each shipment - should leak test each containment boundary prior to each shipment.

Other special design features and appropriate measures before each shipment may be devised and incorporated; however, the acceptability of any features and measures are always at the discretion of the certifying authority.

It is emphasized that watertightness may be a design requirement to ensure subcriticality. How watertightness is achieved, demonstrated before shipment, and maintained during transport conditions are, however, primarily containment and operational issues. Ensuring the integrity of the water-tight boundaries is one of the principal functions of the structural and thermal design requirements.

6.1.3.3 Type A/Type B package

The designation of a package as Type A or Type B is determined by the quantity and type of radionuclides in the contents. A Type A package is required for transporting Type A quantities, and a Type B package is required for Type B quantities. The principal difference between the two is that Type A packages are to be subjected to the normal conditions of transport tests, whereas Type B packages are to be subjected to the normal conditions of transport tests and the hypothetical accident conditions tests. Each type package has specific performance standards (e.g., leak rates, external radiation dose rates, etc.) that must be met. However, if the contents are "fissile," the distinction between Type A and Type B packages becomes meaningless (from the viewpoint of criticality safety) because all packages for fissile material must be subjected to the hypothetical accident conditions tests.

The leak rate criteria for Type B packaging are more stringent than for Type A packaging. The leak rate criteria for Type B packaging are usually sufficient to prevent the leakage of water into the containment vessel. However, as described in the preceding section, if the "exception" is to be approved, an additional containment boundary that meets the watertight criteria leak rate may be required.

6.1.3.4 Other design considerations

As was discussed earlier, the principal impact that nuclear criticality safety has on a package design is the necessity for watertightness of the containment system, which must then be addressed in the chapter on containment. All other aspects of the package design (e.g., structural, thermal, radiation shielding, etc.) usually have a more significant impact on the criticality safety evaluation than the criticality safety concerns have on the other package design considerations.

Water leakage into the containment system is usually a "single-unit" criticality problem. Package designs that satisfy the structural, thermal, and radiation-shielding requirements tend to affect the neutron interaction between packages and therefore are more important in the "array" evaluations. A packaging design that incorporates the following attributes will tend to minimize the neutron interaction between packages in the array:

1. Has a physically small inner container and a large outer container,
2. Has thick-walled inner and outer containers,
3. Structurally is not prone to significant deformation from the drop test,
4. Has a high-density, hydrogenous thermal insulating material, and
5. The thermal insulating material is not prone to significant degradation from the thermal test.

These attributes enhance array subcriticality as a result of neutron absorption in the material of construction; however, they tend to make the package large and heavy, which are undesirable for handling and transporting.

The normal interaction with the structural, thermal, and shielding designers is for the criticality safety analyst to evaluate the design as proposed. Based upon the condition of the package after the normal conditions of transport and hypothetical accident conditions testing, the criticality safety analyst then determines the allowable number of packages that may be transported. If the number of packages allowable for transport is unacceptably small, some of the preceding attributes must be considered in a redesign of the packaging. If the number of packages allowable for transport is acceptable, no additional constraints for criticality safety are necessary.

Although the impact of criticality safety on the design may be minimal, this does not imply that the criticality safety analyst does not need to participate in the design effort. Frequently, the analyst can frequently offer recommendations that have little or no impact on the design but that may significantly enhance the subcriticality of the design. The criticality safety analyst must also participate in the hypothetical accident testing evaluation to adequately assess the damage from the drop, crush, thermal, and submersion tests on the package calculational models.

6.1.4 Definition of Terms

The definitions of the following terms are applicable to this chapter of the guide and may or may not be used in the same context in other chapters of the guide.

Undamaged package - a package that has not been subjected to the normal conditions of transport (NCT) or the hypothetical accident conditions (HAC); it represents the package as offered for shipment.

Damaged package - a package that has been subjected to either the NCT or HAC or both.

Criticality Index (CI) - the dimensionless number determined from the criticality evaluation based upon the 50-unit rule. A CI is determined for both NCT and HAC, and the higher of the two values becomes the CI. The CI will be 0, if and only if, an infinite array of packages is adequately subcritical for both NCT and HAC.

Radiation Index (RI) - the dimensionless number determined from external radiation measurements, that is, the radiation dose rate in mr/h at 1 m (3.3 ft) from the surface of the package.

Transport Index (TI) - the higher of the CI and the RI. The TI is used to limit the number of packages allowed in a transport vehicle and (if not zero) is included on the shipping label.

6.2 REGULATORY REQUIREMENTS FOR NUCLEAR CRITICALITY SAFETY

6.2.1 Regulations

The off-site transportation of fissile and radioactive materials (for both weapons and nonweapons programs) is governed by numerous Department of Energy (DOE) orders, many of which are being revised. Regardless of the state of the order (i.e., approved or draft revision), all DOE orders addressing off-site transportation specify that the packaging either a) meets the safety requirements and performance standards as referenced in Title 10, Part 71^[1] and Title 49, Part 173^[2] of the Code of Federal Regulations (CFR), or b) meets or exceeds the level of safety as compared with the commercial packaging and transportation of fissile and radioactive materials (thereby implying that the CFR requirements and standards are to be met).

The current DOE orders and draft revisions do not cite the specific safety requirements or performance standards but state that the requirements and standards of the CFR shall be met. Therefore, the remainder of this section will identify and discuss the applicable (to nuclear criticality safety) requirements from Title 10 and Title 49 of the CFR.

Title 10 of the CFR, Part 71, "Packaging and Transport of Radioactive Material" (10 CFR 71),^[1] sets forth performance standards and subcriticality requirements that fissile and radioactive material shipping packages must meet. Title 49 of the CFR, Part 173, "Shippers - General Requirements for Shipments and Packaging, Subpart I, Radioactive Materials" (49 CFR 173), sets forth the general

transportation requirements, such as labeling, placarding, and shipment. Title 49, Part 173, also includes (or otherwise references) the requirements of 10 CFR 71^[2] and sets forth additional performance standards for Type A packages not included in 10 CFR 71. However, when the contents are *fissile*, the distinction between Type A and Type B packaging becomes meaningless (only from the standpoint of nuclear criticality safety) because all fissile material packages must meet all the requirements for subcriticality. Proposed rule changes to 10 CFR 71 (see *Federal Register*, Vol. 53, No. 21550, June 8, 1988)^[3] place additional performance standards on certain packages and implement other procedural changes that will affect the nuclear criticality safety evaluation. It is on these proposed rule changes that this chapter of the design guide is based.

6.2.2 General Standards for all Packages

"General Standards for all Packages," (10 CFR 71.43) specifies numerous safety and design requirements, and performance standards applicable to criticality safety, shielding, thermal, structural, containment, and operational aspects of the package. However, this section of the manual discusses only those aspects that the criticality safety analyst should address specifically in the evaluation.

According to 10 CFR 71.43(d), "A package must be of materials and construction which assure that there will be no significant chemical, galvanic, or other reaction among the packaging components or between the packaging components and the package contents, including possible reaction resulting from leakage of water to the maximum credible extent."

The analyst should address (or reference other sections of SARP) the potential for chemical, galvanic, or other reactions that may affect the neutron reactivity of the packaging and contents. If such

reactions are possible, the analysis should evaluate for those conditions that would produce the most reactive configuration or conditions.

6.2.3 General Requirements for Fissile Material Packages

The conditions under which single packages shall remain subcritical are specified in 10 CFR 71.55, "General Requirements for all Fissile Material Packages."

6.2.3.1 Single package, water in-leakage

According to 10 CFR 71.55(b), "Except as provided in paragraph (c) of this section, a package used for the shipment of fissile material must be so designed and constructed and its contents so limited that it would be subcritical if water were to leak into the containment system or liquid contents were to leak out of the containment system so that, under the following conditions, maximum reactivity of the fissile material would be attained: 1) The most reactive credible configuration consistent with the chemical and physical form of the material; 2) Moderation by water to the most reactive credible extent; and 3) Close reflection by water on all sides."

From the standpoint of criticality safety evaluation, 10 CFR 71.55(b) is the most controversial and most emotional issue in the analysis/review process. As stated in Subsect. 6.1.3.1, this regulation is imposed without regard as to how or when the water leakage occurs, the condition of transport, or whether the packaging has been damaged. Only that maximum reactivity is attained to the most reactive credible configuration consistent with the chemical and physical form of the material and moderation by water to the most reactive credible extent. Here in lies the controversy: what is credible in terms of the chemical and physical form of the material when exposed to water, to what extent is water moderation

credible, to what extent do the materials react with the water, what additional physical boundaries are present, and to what extent can credit be taken for these boundaries.

The following specific examples are assumptions that should be acceptable to reviewers.

1. The content is a single piece of metal. The analyst need not assume that the metal *dissolves* in the water such that a theoretical metal-water mixture exists inside the inner containment vessel. In this case, the single metal piece is full water reflected. NOTE: This approach may not be acceptable if the metal (e.g., in some alloy) reacts with the water or if the water is *significantly* corrosive to the metal (such as sea water).
2. The contents are multiple pieces of metal. The analyst should determine optimum spacing of the metal pieces within the flooded inner containment vessel to produce maximum reactivity. Except as noted in Example 1, the metal does not need to be dissolved in the water.
3. The contents are a powder. The analyst should assume that the powder is a theoretical powder-water mixture (e.g., oxide-water) and determine the maximum reactivity for various mixtures. This determination will include varying the hydrogen-to-fissile material atomic ratio (H/X) of the mixture and the volume/geometry of the mixture to determine maximum reactivity.
4. The contents are also packaged in a secondary container (e.g., a plastic bottle, a mechanically sealed can, etc.) that is placed in the inner containment vessel. The analyst must evaluate for maximum reactivity (as described in Examples 1, 2, and 3) within the volume of this secondary container. However, the analyst must address the adequacy of the secondary container integrity to contain the material under all conditions. For example, does the plastic bottle melt or deform

from thermal tests, and is sufficient shock absorbing material provided to prevent damage from drop tests? In other words, if the analyst takes credit for the limited volume of the secondary container, justification of the assumption must be provided; otherwise, the total volume of the containment vessel should be considered (as described in Example 3).

5. The contents include a material (in addition to the fissile material) that has very high neutron absorption characteristics and this material is soluble (or chemically reacts) in water. The principal (and most difficult) issue to address is the credibility of the dissolved neutron absorber escaping the containment. On one hand, the regulations require that in-leakage of water be considered, and it is only logical to consider that it can also leak out, taking the dissolved neutron absorber with it. On the other hand, if the containment remains watertight, the analyst must consider water in-leakage (a regulatory requirement) but does not have to consider subsequent outleakage— if it has been adequately demonstrated that containment remains watertight during all normal and accident conditions. If one can defend not considering outleakage, the evaluation may still need to consider redistribution of the neutron absorber to adhere to the regulatory requirement that maximum reactivity of the fissile material be attained.
6. The fissile material is a solid metal but reacts (or dissolves) with water. To satisfy the water in-leakage requirement, metal-water mixtures should be evaluated. Assuming that the maximum reactivity of the fissile material is critical, the only available option is to pursue an exception to the water in-leakage requirement.

As was stated earlier, 10 CFR 71.55(b) says that the package must remain subcritical under the assumed conditions. If the proposed contents in a single package are adequately subcritical for the assumed water leakage conditions, the analyst may proceed to the next step of the evaluation. However,

if the proposed contents in a single package (for the assumed conditions) are not adequately subcritical, the following three options are available: 1) reduce the quantity of contents and/or reduce the dimensions of the containment system, 2) add neutron poisons to the fissile material, 3) pursue an exception to the water in-leakage requirement. The first two options which were discussed in Subsect. 6.1.3.1, will not be repeated.

According to 10 CFR 71.55(c), "The Commission may approve exceptions to the requirements of paragraph (b) of this section if the package incorporates special design features that ensure that no single packaging error would permit leakage, and if appropriate measures are taken before each shipment to ensure the containment system does not leak."

Option 3, an exception to the water in-leakage requirement, may be approved by the certifying authority if the package design incorporates special features that ensure that no single packaging error would permit leakage and if appropriate measures are taken before each shipment to ensure that the containment system does not leak. The adequacy of the special design features and the appropriate measures before each shipment have been a source of considerable controversy.

The following are generally considered necessary to satisfy these two requirements:

1. Special features - should include multiple containment boundaries, each meeting the minimum leak rate criteria (e.g., watertightness), each containment boundary is leak rate testable, and each containment boundary remain watertight after being subjected to the hypothetical accident conditions tests, and

2. Appropriate measures before each shipment - should leak test each containment boundary prior to each shipment.

Other special design features and appropriate measures before each shipment may be devised and incorporated; however, the acceptability of any features and measures is always at the discretion of the certifying authority.

A philosophy gaining general support in the nuclear criticality safety community is initially to design and fabricate the package with multiple water-tight boundaries such that the exemption provided in 10 CFR 71.55(c) could be approved (if the boundaries remain watertight after testing). Then it would be unnecessary for the analyst to waste time and effort evaluating water in-leakage conditions as was discussed earlier. This concept, if acceptable to the package certifying authority, would be very useful, especially when the package contents contain water-soluble neutron absorbers. Although this philosophy is technically defensible, it has not yet been attempted.

6.2.3.2 Single package, normal conditions of transport

According to 10 CFR 71.55(d), "A package used for the shipment of fissile material must be so designed and constructed and its contents so limited that under the tests specified in 71.71 (NCT): 1) The contents would be subcritical; 2) The geometric form of the package contents would not be substantially altered; 3) There would be no leakage of water into the containment system unless, in the evaluation of undamaged packages under 71.59(b)(1), it has been assumed that moderation is present to such an extent as to cause maximum reactivity consistent with the chemical and physical form of the material; and 4) There will be no substantial reduction in the effectiveness of the packaging, including: 1) No more than five percent reduction in the total effective volume of the packaging on which nuclear safety is assessed;

2) No more than five percent reduction in the effective spacing between the fissile contents and the outer surface of the packaging; and 3) No occurrence of an aperture in the outer surface of the packaging large enough to permit the entry of a 10-cm (4 in.) cube."

These requirements are directed at the evaluation for a single package that has been subjected to the Normal Conditions of Transport tests described in 10 CFR 71.71. Of these requirements, Parts 71.55(d)(1) and 71.55 (d)(2) specify conditions that the criticality analyst must evaluate. The effects of temperature variations, described in 10 CFR 71.71(b) and (c), on the neutron cross sections must be included in the evaluation. Common practice however, is to combine the evaluation of temperature effects in the section addressing hypothetical accident conditions because higher temperatures usually occur from the thermal testing.

Except as described herein, the other requirements of 10 CFR 71.55(d) specify physical design criteria that the package must be shown to meet, and which are generally addressed in other chapters of SARP (e.g., structural, containment, shielding, thermal, etc.). However, it is suggested that a summary of the results from these other chapters be provided in the criticality chapter for completeness and justification of the conditions that the criticality analyst is evaluating.

6.2.3.3 Single package, hypothetical accident conditions

According to 10 CFR 71.55(e), "A package used for the shipment of fissile material must be so designed and constructed and its contents so limited that under the tests specified in 71.73 (HAC), the package would be subcritical. For this determination, it must be assumed that: 1) The fissile material is in the most reactive credible configuration consistent with the damaged condition of the package and the chemical and physical form of the contents; 2) Water moderation occurs to the most reactive credible

extent consistent with the damaged condition of the package and the chemical and physical form of the contents; and 3) There is reflection by water on all sides, as close as is consistent with the damaged condition of the package."

These requirements are directed at the evaluation of a single package which has been subjected to the Hypothetical Accident Conditions tests described in 10 CFR 71.73. The analyst must consider the damage suffered by the package from the drop and puncture tests, the thermal test, and the immersion test. Other chapters in SARP describe the results of these tests; however, a summary of the results should be provided in the criticality chapter for completeness and justification of the conditions that the criticality analyst is evaluating.

Any reactivity calculations performed on the single damaged package are normally considered an extension of the reactivity calculations performed on the single undamaged package. The principal importance and criticality concerns usually develop when the packages (undamaged and damaged) are evaluated in arrays.

6.2.4 Standards for Arrays of Fissile Material

The proposed rule changes to 10 CFR 71 (see *Federal Register*, Vol. 53, No. 21550, June 8, 1988)^[3] eliminate the three fissile classes and make minor changes in how to determine the transport index. The following discussion considers the proposed rule changes.

According to 10 CFR 71.59(a), "A fissile material package must be controlled by either the shipper or the carrier during transport to assure that an array of such packages remains subcritical. To enable this control, the designer of a fissile material package shall derive a number 'N' based on all the

following conditions being satisfied, assuming packages are stacked together in any arrangement and with close reflection on all sides by water: 1) Five times 'N' undamaged packages with nothing between the packages would be subcritical; 2) Two times 'N' damaged packages, if each package were subjected to the tests specified in 71.73 (HAC) would be subcritical with optimum interspersed hydrogenous moderation; and 3) The value of 'N' cannot be less than 0.5." The number "N" is used to determine the TI, and N should be determined for NCT and HAC.

6.2.4.1 Normal conditions of transport

Item (1) of Part 71.59(a) requires that a water-reflected array of "undamaged packages with nothing between the packages" be evaluated. The term *undamaged package* means the package as offered for shipment. The analyst must address various array sizes and different stacking arrangements of packages in the evaluation.

If an infinite array of undamaged packages is adequately subcritical, it is usually unnecessary to evaluate water-reflected finite arrays. Note: infinite arrays are not water reflected. However, if the neutron leakage from a single, undamaged package is significant, there will be neutron interaction between packages, and then array size and perhaps package orientation will become important. The objective is to determine the maximum number of undamaged packages that are subcritical; the value of "N" for the normal conditions of transport is 1/5 the maximum subcritical number.

6.2.4.2 Hypothetical accident conditions

Item (2) of Part 71.59(a) requires that a water-reflected array of "damaged packages, if each package were subjected to the tests specified in Part 71.73," be considered. The term *damaged package* requires that the analyst address all possible damage conditions resulting from the HAC testing.

Specific damage conditions most important to the criticality safety evaluation include (but are not limited to) the following: 1) reconfiguration of the fissile material contents, 2) water leakage into the containment vessel, 3) change in external dimensions of the outer container (affecting spacing of the fissile contents), 4) degradation of the thermal insulation, and 5) water leakage into the outer container. To determine maximum reactivity, the variations in package damage must be addressed for different array sizes with optimum water moderation between the packages.

The objective is to determine the maximum number of damaged packages that are subcritical under the most reactive, most credible accident conditions. The value of "N" for the hypothetical accident conditions is 1/2 the maximum subcritical number.

6.2.4.3 Calculation of the transport index

According to 10 CFR Part 71.59(b), "The transport index based on nuclear criticality control shall be obtained by dividing the number 50 by the value of "N" derived using the procedures specified in paragraph (a) of this section. The value of the transport index for nuclear criticality control may be zero provided that an unlimited number of packages is subcritical such that the value of "N" is effectively equal to infinity under the procedures specified in paragraph (a) of this section. Any transport index greater than zero must be rounded up to the first decimal place."

A TI must be determined for each condition, that is, for an array of undamaged packages representing normal conditions of transport and for an array of damaged packages representing the most reactive hypothetical accident conditions. In equation notation,

$$TI_{NCT} = \frac{50}{N_U} = \frac{50}{1/5 X_U} = \frac{250}{X_U}$$

$$TI_{HAC} = \frac{50}{N_D} = \frac{50}{1/2 X_D} = \frac{100}{X_D}$$

where

N_U = the number of packages that may be shipped based upon NCT criteria,

N_D = the number of packages that may be shipped based upon HAC criteria,

X_U and X_D = the maximum number of packages determined to be subcritical for undamaged conditions (U) and damaged conditions (D), respectively; $N_U = 1/5 X_U$, and $N_D = 1/2 X_D$.

The higher of these two TI values becomes the transport index for purposes of criticality control. The TI as determined above for criticality safety purposes will be 0, if and only if, the values of X_U and X_D are "effectively equal to infinity."

6.2.4.4 Special requirements for plutonium

The proposed rule changes^[3] have included additional requirements for plutonium packages. These changes include 10 CFR 71.63, "Special Requirements for Plutonium and Other High-Toxicity Radionuclide Shipments;" 10 CFR 71.64, "Special Requirements for Plutonium Air Shipments;" 10 CFR 71.74, "Plutonium Accident Conditions;" and 10 CFR 71.88, "Air Transport of Plutonium."

These additional requirements for plutonium have no direct impact on the criticality safety evaluation discussed earlier, except that the plutonium accident conditions may damage the package more severely than the usual hypothetical accident conditions. As was stated earlier, the criticality safety analyst must participate in the accident testing evaluation to assess adequately the damage from the drop, crush, thermal, and submersion tests on the package calculational models.

6.2.4.5 Transportation control requirements

According to 10 CFR 71.59(c), "Where a fissile material package is assigned a nuclear criticality control transport index - 1) Not in excess of 10, that package may be shipped by any carrier, and that carrier provides adequate criticality control by limiting the sum of the transport indexes to 50 in a non-exclusive use vehicle and to 100 in an exclusive use vehicle. 2) In excess of 10, that package may only be shipped by exclusive use vehicle or other shipper controlled system specified by DOT for fissile material packages. The shipper provides adequate criticality control by limiting the sum of the transport indexes to 100 in an exclusive use vehicle."

These controls are not a part of the criticality design or evaluation process but are an integral part of fissile material shipping regulations. Paragraph (c) is included here because it is a part of the overall

nuclear criticality safety control requirements. The reference to "DOT" in Item (2) directs the shipper to 49 CFR Part 173, "Shippers - General Requirements for Shipments and Packaging, Subpart I, Radioactive Materials" (49 CFR Part 173.401 through Part 173.478).

6.3 CALCULATIONAL MODELS - DIMENSIONAL

6.3.1 General

Modeling an exact representation of the shipping packaging and its contents is usually impossible and unnecessary. The calculational models however, that are developed, must be of sufficient detail to describe explicitly the physical features that are important to the nuclear criticality calculations. Simplified, dimensioned figures depicting the physical features modeled in the calculations should be provided. Figures drawn specifically for the various portions of the model are preferable to providing the engineering drawings (which are usually provided in Sect. 1 of SARP). It is generally simpler and clearer to limit the dimensional features provided on each figure and to provide multiple figures with each figure building on the preceding figure.

It is often useful to provide four types of calculational models: 1) the contents model, 2) the inner container model, 3) the single package model, and 4) the array package model. The contents model may include all geometric and material regions out to the primary containment boundary or any other convenient boundary. This model then dimensionally fits inside the single package model and the array package model. Multiple figures may be required for each calculational model to show adequately yet simply the necessary detail. Multiple figures may be necessary for the contents model to show different loading options and for the array packaging model to depict different types of damaged conditions. The dimensions provided on each figure should be the values used in the geometry input for the calculations.

Each calculational model should include a table identifying the material in each region of the model. It is useful to provide in this table additional information such as the density, the region mass represented by the model, and the actual mass of the region. The dimensions, materials, and masses provided in the figures must be comparable to and consistent with the corresponding items in the engineering drawings, and should be the same numerical values used in the input of the calculational method. Frequently, the reference drawings and specifications for the packaging use the English system of measurement (inches, feet, and pounds) rather than the metric system (centimeters and grams) typically required as input to neutronic computer codes. When both systems of measurement are encountered, both values should be included when discussing them in the text whereas only the metric values as used in the computer code input are needed in tables and figures.

Associated with each figure should be a subsection describing that portion of the model. Differences between the calculational models and the as-shipped configuration should be identified and discussed. The discussion should state why there is a difference, how the different value was determined, and the impact of the calculational results (i.e., conservative or nonconservative).

Dimensional tolerances of the packaging and contents should be addressed. When the calculational models are being designed, tolerances that tend to add conservatism (i.e., produce higher neutron multiplication factors) should be included. For some situations, it may be necessary to evaluate the effects of including the maximum, as opposed to the minimum, tolerances. For example, the steel wall of a drum-type container will function as a neutron reflector for a single package but will function as a neutron absorber in an array of packages. Adding the plus tolerance to the nominal wall thickness may be conservative for single package calculations but may be nonconservative for array calculations.

The nuclear criticality evaluation is required to address normal conditions of transport and hypothetical accident conditions with specific requirements for both single packages and for an array of packages. By judiciously developing the calculational models representing the as-shipped configuration, one can minimize the number of different models necessary to analyze normal and accident conditions. If no significant dimensional changes are caused by accident conditions, material changes (such as water flooding and reflection) and the number of packages in an array may be the only variables that require investigation. If significant dimensional changes (e.g., contents shifting in the inner cavity of the packaging or external deformation affecting spacing) are necessary, additional calculational models and figures may be needed.

6.3.2 Example Model Description

To illustrate the calculational model features described in this section and the materials aspects described in Sect. 6.4, a fictitious shipping package (described in this section) will be used. The package and its contents are completely fictitious and do not represent certified container loadings or configurations.

This simple example is provided to demonstrate the degree of detail that should be included in the criticality evaluation. The format of the text generally follows the standard format required for SARP preparation as described in the U. S. Nuclear Regulatory Commission (NRC) Regulatory Guide 7.9.^[4] In an actual SARP, all sources of information and data should be referenced as to its origin. However, in the interest of simplicity, the references are not included in the example.

Fictitious shipping package model FSP-30 uses a Department of Transportation (DOT) Specification 17C, 30-gallon steel drum [American National Standards Institute (ANSI)/ASC M42] as the

confinement boundary. The drum body and head sheets are made of 18-gauge low-carbon steel. Two approximately equally spaced rolling hoops are swaged into the drum body. The removable head sheet is closed by a 12-gauge bolted ring clamp. The drum is lined with industrial cane fiberboard (ASTM C-208), which provides thermal insulation, vibration and shock isolation, and central positioning of an inner container within the drum. The insulation provides a minimum thickness between the inner container and the drum of 5 ¾ in. radially and 4 in. axially (top and bottom) and has a density of 15 lb/ft.³ The watertight inner container constitutes the containment boundary. The containment vessel wall is made of 6-in. Schedule-40 carbon-steel pipe [ANSI/American Society of Mechanical Engineers (ASME) B36.10M]. One end of the inner container is sealed with a standard butt weld ellipsoidal pipe cap and the removable end is closed with a standard screw-type pipe cap. The model FSP-30 shipping container may be used to transport the following forms of uranium enriched to 93.5 wt % in the ²³⁵U isotope:

14.438 kg uranium as metal, H/U* = 0,

10.802 kg uranium as a dry compound, UH₃, H/U = 3.

The uranium metal consists of a cylindrical rod 7.62 cm diameter by 16.8768 cm high. The metal rod is wrapped in a bubble-pack cushioning material when it is placed into the inner container. The uranium compound consists of a solid uranium hydride (UH₃) rod 10.16 cm diameter by 12.3246 cm high. The UH₃ rod is wrapped in a bubble-pack cushioning material when it is placed into the inner container.

*H/U is the ratio of hydrogen atoms to uranium atoms.

6.3.3 Contents Model

The contents model depicts the contents to be placed in the packaging. If different loading configurations (including partial load configurations) are to be included, a model depicting each loading should be provided, although it may be possible to develop and justify a single contents model that will encompass different loading configurations.

6.3.3.1 Contents model example

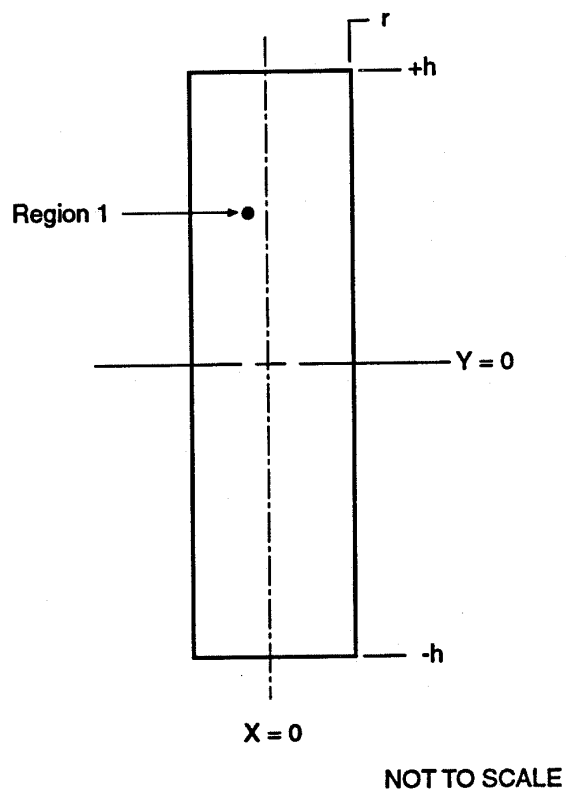
Based on the description in Subsect. 6.3.2, an example of the contents model is developed and shown in Subsects. 6.3.3.1.1 and 6.3.3.1.2. In this example, the contents model is comprised of a fuel configuration model and an inner container model.

Fuel configuration calculational model example

Figure 6.1 depicts a cross section of the fuel configurations used in the calculations. The figure includes a table that provides a complete physical description of the two fuel configurations.

Inner container calculational model example

Figure 6.2 depicts a cross section of the inner container calculational model. The figure includes a table identifying the regions, materials, material densities, modeled mass as used in the calculations, and actual mass.

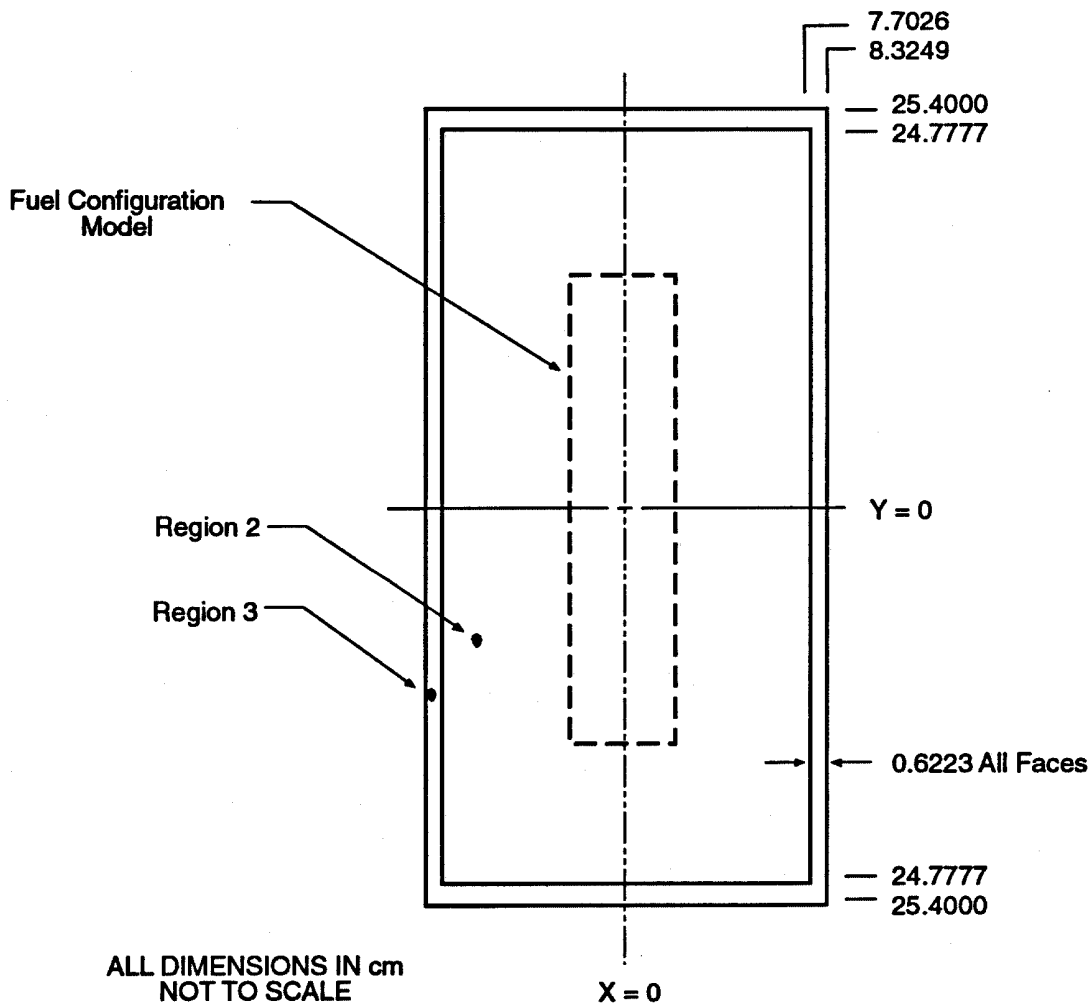


Region	Fuel Material ^a	r (cm)	± h (cm)	Material density g/cm ³	Uranium density gU/cm ³	Mass U (g)
1	Metal	3.8100	8.4384	18.7600	18.7600	14,438.5
1	Dry compound	5.0800	6.1623	10.9500	10.8111	10,802.4

^aUranium fuel at an enrichment of 93.5 wt % ²³⁵U.

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Fig. 6.1. Fuel configuration calculational models.



Region	Material	Density (g/cm ³)	Model Mass (g)	Actual Mass (g)
2	Polyethylene	0.1500	various (see text)	a
3	Carbon steel	7.8212	14,263.9	a

^a Actual mass from packaging description section would go here.

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Fig. 6.2. Inner container calculational model.

The inner container is modeled as a straight-wall, right circular cylinder with uniform wall thickness on the top, bottom, and sides. The model differs from the actual inner container in that the top and bottom are taken to be flat plates with the same thickness as the side wall. The cylindrical part of the inner container is constructed from 6 in. Schedule-40 pipe. From standard pipe schedule tables, the outside diameter is 6.625 in. and the inside diameter is 6.065 in. with a wall thickness of 0.280 in. Because standard pipe has a 12.5% mill tolerance on the wall thickness, it is reduced to 0.245 in. Therefore, the inner container model is 6.135 in. inside diameter (7.79 15 cm inside radius), 6.625 in. outside diameter (8.4138 cm outside radius), with a wall thickness of 0.245 in. (0.6223 cm).

Because the actual inner container has an elliptical bottom and the model has a flat bottom, the model inside height was adjusted to conserve the actual inside volume. (Note: in an actual package evaluation, the actual inner container height and volume values should be included in this section.) Therefore, the inside height of the model is 49.5554 cm, resulting in an inside volume of 9236.7 cm³. With the top and bottom thicknesses of 0.6223 cm, the outside height of the model is 50.8000 cm.

6.3.4 Single Package Calculational Model

The single package model with the contents model depicts the as-shipped configuration of the packaging and contents and is used for the single package calculations required by 10 CFR 71.55(b).

6.3.4.1 Single package calculational model example

Based on the description in Subsect. 6.3.2, an example of the single package model is developed and shown as follows.

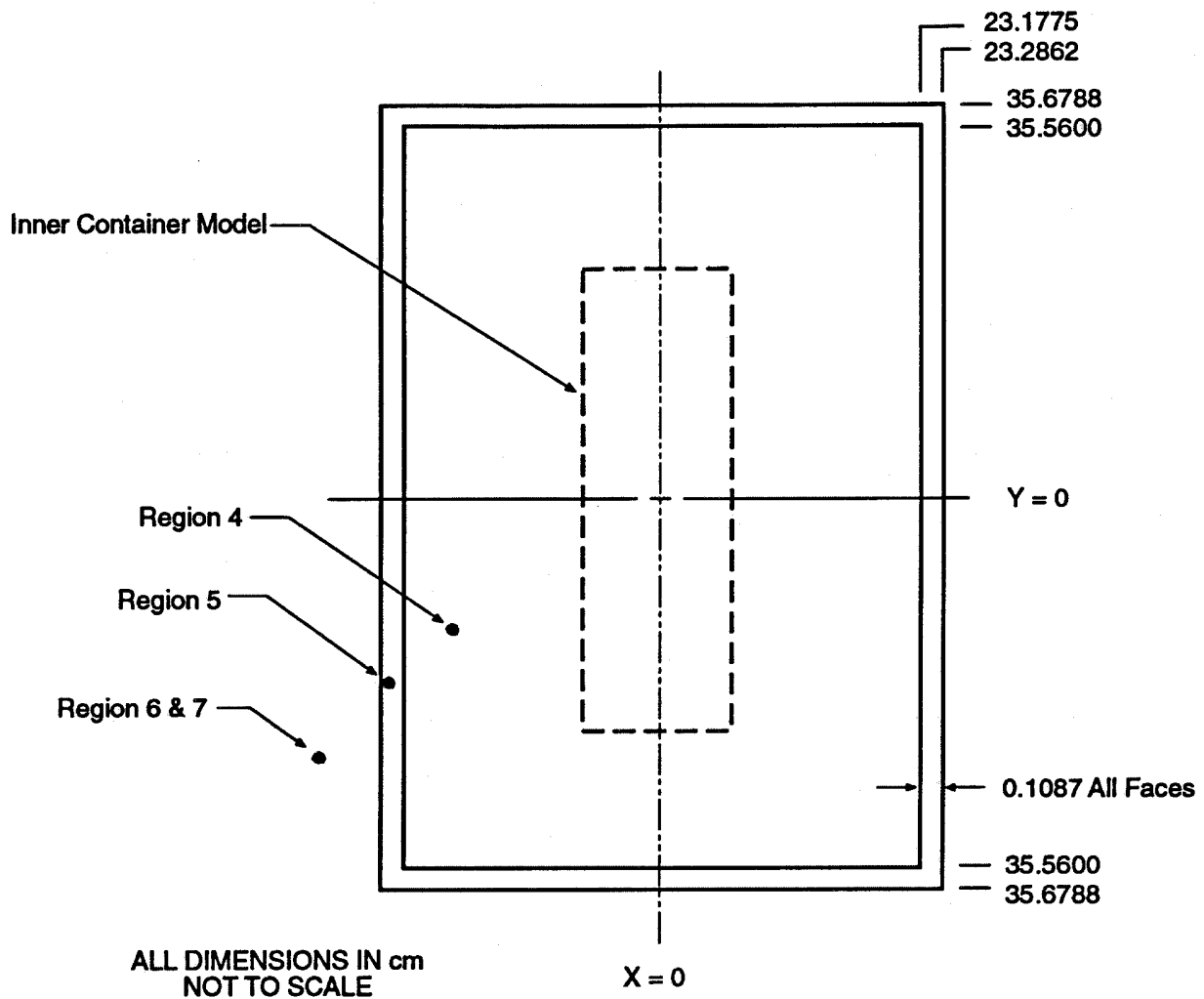
Figure 6.3 depicts a cross section of the single unit packaging calculational model. The figure includes a table that identifies regions, materials, material densities, modeled mass as used in the calculations, and actual mass.

The outer DOT Specification 17C drum is modeled as a straight-wall, right-circular cylinder with a uniform wall thickness on the side, top, and bottom. The inside diameter is 18 1/4 in. (23.1775 cm inside radius), and the inside height is 28.0 in. (71.1200 cm inside height). The drum wall, top, and bottom are 18-gauge steel, nominally 0.0478 in. thick. The wall, top, and bottom are modeled as 0.0428 in. (0.1087 cm) thick, which is the minimum specification for 18-gauge steel per 49 CFR 178.115, Specification 17C. Therefore, the outside radius is 23.2862 cm, and the outside height is 71.3374 cm.

The single unit packaging model of the 30-gallon drum differs from the actual Specification 17C drum in the treatment of the drum wall, which is modeled as a straight wall cylinder without the rolling hoops. The model also does not have the top and bottom inset into the drum wall, and the minimum thickness specification is used for the drum top, bottom, and side. (Note: in an actual packaging evaluation, the actual drum mass should be included in the discussion.)

6.3.5 Array Package Model

Most package designs are cylindrical, often based on use of a drum for the outside layer of the package. Collections of cylindrical packages may be arranged either intentionally or by accident conditions into a triangular-pitch configuration. The array density for a triangular-pitch arrangement is about 15.5% greater than that for a square-pitch configuration. While some computer codes permit modeling triangular-pitch lattices, the geometry input can be unwieldy, and may be difficult to make simple changes necessary for parametric variations. To avoid the difficulties of modeling triangular-pitch



Region	Material	Density (g/cm ³)	Model Mass (g)	Actual Mass (g)
4	Thermal insulation	0.2403	26,184.4	a
5	Carbon steel	7.8212	11,722.0	a
6 & 7	Water or void	variable	variable	variable

^aActual mass from packaging description section would go here.

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Fig. 6.3 Single-unit packaging calculational model (full-diameter model).

arrangements of packages, the outside diameter of the single package model can be reduced by 7% to create the array package model. This 7% reduction in diameter produces an array density for the square-pitch lattice equal to the array density of a triangular-pitch lattice of packages with the original diameter. It can be shown that the diameter reduction of square-pitch lattice packages is no more reactive than the true diameter packages in a triangular-pitch configuration.

The diameter reduction will reduce the volume, and consequently the mass, of material in each region where the diameter is altered. Diameter reduction should not be applied to either the contents model or the inner container model. The regional volume reduction of the array package model may be addressed by either of two methods. The first method is to select a region for which the reduction in mass will be conservative for the array calculations. A thick radiation shielding region would be an example. The evaluation must also demonstrate that this regional mass reduction is not nonconservative compared with the single package model calculations. The second method is to select a region that contains a less than full density material, such as a region of low-density thermal insulation, and to increase the density in the calculations to conserve the actual mass.

The diameter reduction technique or triangular pitch modeling is not necessary for shipping packages that exhibit little or no neutron interaction. This condition is often observed for heavily shielded spent fuel casks. If the neutron leakage fraction from a single unreflected package is less than about 0.25, neutron interaction between packages in an array will usually be insignificant. The best measure of neutron interaction is to compare the calculated k_{eff} of a single package with that of an infinite array of packages. If the single package k_{eff} is within a few percent of the infinite array factor, k_{∞} , neutron interaction is not a concern, and one may conclude that package spacing is not a sensitive parameter. For such packages, use of the full diameter, single package model is justifiable for all array calculations,

and there is no need to use either triangular-pitch modeling or the diameter reduction technique to account for triangular-pitch configurations of packages.

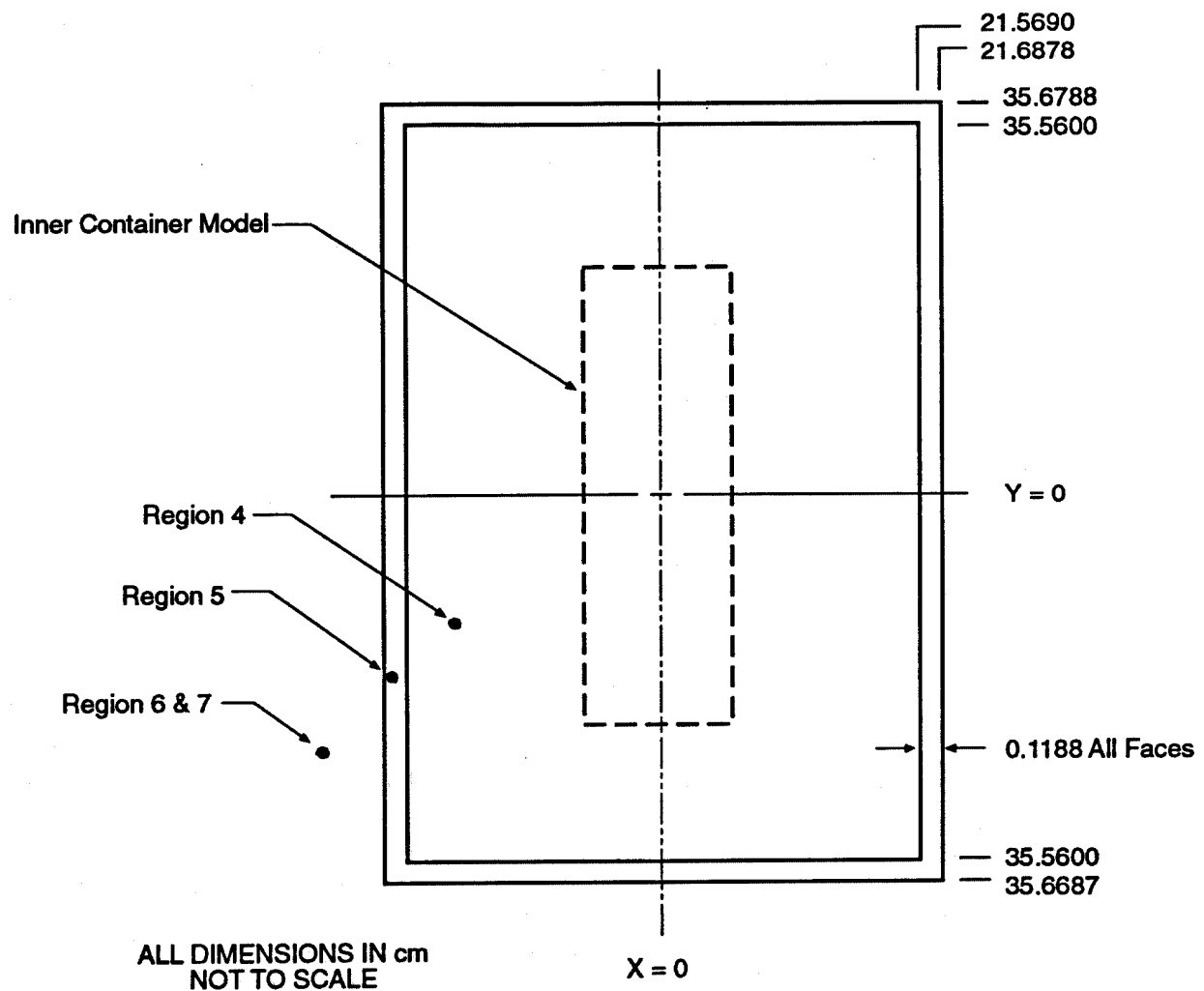
6.3.5.1 Array package calculational model example

Based on the description in Subsect. 6.3.2, an example of the array package model is developed and shown as follows.

For cylindrical containers, array density is maximized when they are arranged in a triangular-pitch configuration. The FSP-30 may be shipped in a triangular-pitch configuration, or such a configuration may occur as a result of accident conditions. To avoid modeling relatively complex triangular-pitch arrays, a square-pitch array can be modeled to emulate a triangular-pitch array by reducing the outside diameter of the package by 7%. The reduction in diameter for a square-pitch configuration maintains the same fissile unit density within the array as the full-diameter packaging in triangular-pitch configuration. Conserving the steel mass in the outer DOT Specification 17C drum and the mass of the industrial cane fiberboard thermal insulation results in neutron interaction rates within the array that are essentially identical. To conserve the mass of steel, the drum wall thickness must be increased; to conserve the mass of thermal insulation, the density must be increased.

Figure 6.4 depicts a cross section of the array package model. The figure includes a table that identifies regions, materials, material densities, modeled mass as used in the calculations, and the actual mass.

The array package model differs from the single package model in that the inside diameter of the array package model drum has been reduced by 6.903% to 43.1380 cm (21.5690 cm radius). The inside



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Region	Material	Density (g/cm ³)	Model Mass (g)	Actual Mass (g)
4	Thermal insulation	0.2819	26,184.0	a
5	Carbon steel	7.8212	11,706.4	a
6 & 7	Water or void	variable	variable	variable

^aActual mass from packaging description section would go here.

Fig. 6.4 Array-packaging calculation model (reduced-diameter model).

height remains 71.1200 cm. The uniform wall thickness is determined by maintaining the single package model drum mass of 26,184.4 g. The resulting wall thickness is 0.1188 cm. Therefore, the outside radius of the array package model is 21.6878 cm and the outside height is 71.3576 cm. With these dimensions, the steel mass as modeled is 26,184.0 g. The slight differences between the masses between the single package and the array package models is the result of computational roundoff when determining the wall thickness. (Note: in an actual packaging evaluation, any structural damage, packaging volume reduction, etc., from testing to the hypothetical accident conditions would be included in this subsection.)

6.4 CALCULATIONAL MODELS - MATERIALS

6.4.1 General

Each figure showing a portion of the calculational model should have a corresponding discussion detailing the material compositions and densities of each material region identified in the figure. If standard or code default densities are used, the values should be stated. If densities other than normal are used, the discussion should state why the density is different and how the altered density was determined. For example, if dimensional differences between a region in the calculational model and the as-shipped configuration result in a significant volume difference in that region, it may be necessary to adjust the material density to conserve the actual mass. Composition differences should also be discussed and justified. For example, a ligneous fiber thermal insulating material may be compositionally represented as cellulose at the same density.

Material specifications and associated tolerances should be addressed. When developing the input data for materials, the material parameters should be either maximized or minimized to produce

conservative results. As an example, fissile constituents should be maximized and neutron-absorbing constituents should be minimized.

A summary table should be included identifying all regions in the calculational models and specifying for each region the material, density, constituents, and the weight fraction or percentage and atomic density of each constituent.

6.4.2 Package Regional Densities Example

Based on the description in Subsect. 6.3.2, an example is developed and shown in the next four subsections.

6.4.2.1 Material compositions used in the fuel configuration model (Fig. 6.1)

Two different fuel compositions were used in the calculations as shown in Fig. 6.1 and Table 6.1. In each fuel, the fissile material is uranium enriched to 93.5 wt % in the ^{235}U isotope. The fuel is taken to be a mixture of the ^{235}U and ^{238}U isotopes; i.e., neither nonuranium impurities nor the ^{234}U and ^{236}U isotopes are considered to be present. The metal fuel has a density of 18.76 g U/cm^3 and a hydrogen-to-uranium (H/U) atomic ratio of zero. The dry compound fuel is uranium hydride (UH_3) at a density of $10.95 \text{ g UH}_3/\text{cm}^3$ and an H/U ratio of 3.

For each of the two fuel compositions, Table 6.1 presents the material density, constituents, weight percentage, and atomic density of each constituent used in the calculations. (Note: any differences between the compositions as modeled and the compositions as shipped would be described in this section.)

Table 6.1. Fuel compositions used in calculations

Region for Fig. 6.1	Fuel type	Density (g/cm³)	Constituent	Weight percent	Atomic density (atoms/b cm)
1	Metal	18.7600	²³⁵ U	93.5000	4.4941-2 ^a
			²³⁸ U	6.5000	3.0848-3
1	Dry compound	10.9500	²³⁵ U	92.3135	2.5899-2
			²³⁸ U	6.4175	1.7777-3
			H	1.2690	8.3033-2

^a Read as 4.4941 x 10⁻²

6.4.2.2 Material composition used in the inner container calculational model (Fig. 6.2)

The compositions of materials used in the inner container calculational model are presented in Table 6.2 as Regions 2 and 3. Region 2 represents a low-density (0.1500 g/cm^3) polyethylene (sometimes referred to as "bubble pack") used to cushion and center the uranium metal and dry compound fuel loadings in the inner container. Region 3 represents the steel container. The material is the default carbon steel provided by the SCALE Standard Composition Library. (Note: any other differences between the compositions as modeled and as actually exist would be discussed in this section.)

6.4.2.3 Material compositions used in the single package calculational model (Fig. 6.3)

The material compositions used in the single package calculational model are presented in Table 6.2 as Regions 4a, 5, 6, and 7. Region 4 represents the thermal insulation that is industrial cane fiberboard. This material is taken to be cellulose ($\text{C}_6\text{H}_{10}\text{O}_5$) at a density of 15 lb/ft^3 (0.2403 g/cm^3). Region 5 represents the 30-gallon steel drum with the composition being the default carbon steel from the SCALE Standard Composition Library. Regions 6 and 7 are outside the drum with Region 6 representing variable-density water to model interstitial moderator and Region 7 representing a full-density water reflector when used. (Note: any other differences between the composition as modeled and as actually exists would be discussed in this section.)

6.4.2.4 Material compositions used in the array package calculational model (Fig. 6.4)

The material compositions used in the array package calculational model are presented in Table 6.2 as Regions 4a, 5, 6, and 7. Region 4a represents the thermal insulation with the density adjusted to conserve the insulation mass from the single package calculational model. Based upon the

Table 6.2. Other material compositions used in calculations

Region	Material	Density (g/cm ³)	Constituent	Weight percent	Atomic density (atoms/b cm)
2	Polyethylene	0.1500	H	14.3811	1.2890-2 ^a
			C	85.6189	6.4451-3
3	Carbon steel	7.8212	C	1.0000	3.9250-3
			Fe	99.0000	8.3498-2
4	Insulation (Fig. 6.3.4.1-3)	0.2403	H	6.2189	8.9298-3
			C	44.4294	5.3579-3
			O	49.3517	4.4649-3
4a	Insulation (Fig. 6.3.5.1-4)	0.2819	H	6.2189	1.0476-2
			C	44.4294	6.2854-3
			O	49.3517	5.2378-3
5	Carbon steel	7.8212	C	1.0000	3.9250-3
			Fe	99.0000	8.3498-2
6 & 7	Water	0.9982 ^b	H	11.1909	6.6751-2
			O	88.8091	3.3376-2

^a Read as 1.2890×10^{-2} .

^b Water density in Region 6 varied to simulate different degrees of interstitial moderator.

dimensions and density of Region 4 in Fig. 6.3, the mass of insulation is 26,184.4 g. Using this mass and the dimensions of Region 4a from Fig. 6.4, the density is calculated to be 0.2819 g/cm³. The material compositions in Regions 5, 6, and 7 are the same as in the single package calculational model. (Note: in a real packaging evaluation, additional material composition data would be required to address, for example, degradation of thermal insulation resulting from thermal testing.)

6.4.3 Neutron Absorbers

All materials exhibit some degree of neutron absorption characteristics. Criticality calculations must take credit for the neutron absorption in fissile material to demonstrate subcriticality. Traditionally, neutron-absorbing materials are divided into two categories: materials of construction and neutron poisons.

Materials of construction include all materials normally present, such as the steel in the inner and outer containers, the thermal insulation, the packing material, etc., and also includes the fissile material itself. These materials are usually guaranteed always to be present by virtue of their function. Neutron poisons, on the other hand, are intentionally added, specifically for the purpose of absorbing neutrons to reduce neutron reactivity or to limit neutron reactivity increases during abnormal conditions. Therefore, special attention is always required to guarantee both its presence and the proper distribution of the neutron- absorbing material.

The difference between materials of construction and neutron poisons may be only conceptual and may be defined only by the purpose of its presence; however, a criticality safety evaluation usually does not make a distinction between the two materials. A thorough criticality evaluation will obviously address the effectiveness of the neutron absorption properties of all the materials under both normal and accident

conditions (e.g., changes in neutron absorption cross sections as a function of temperature, neutron energy spectrum, the distribution of the absorbing materials for different accident conditions, etc.).

The principle concern with relying on neutron absorption by poisons (as opposed to relying on neutron absorption by the materials of construction) is ensuring its presence. Omitting a required neutron poison during package loading may be a credible contingent condition not addressed in the evaluation, because it is a container loading issue and not a transportation hypothetical accident condition. If the criticality evaluation determines that a neutron poison is required to ensure subcriticality (refer to Option 2 in Subsect. 6.1.3.1), the analyst must ensure that the appropriate requirements are included in the packaging operations, acceptance testing and maintenance, and quality assurance chapters of SARP (usually Chaps. 7, 8, and 9, respectively).

When neutron poisons are necessary for reasons of subcriticality, it is advisable to incorporate them into the normal materials of construction. For example, a borated steel could be used for the inner container to reduce the neutron interaction between packages, provided it is structurally/thermally acceptable, or cadmium could be plated on the inside surface of the inner container. These examples are techniques that will reduce the probability that the absorbers will be omitted during packaging operations. However, verifying (and reverifying at some frequency) that the absorbers are indeed present, in the prescribed quantity and distribution could present significant problems of operations and quality assurance.

When highly effective neutron-absorbing materials are an integral part of the contents to be shipped, they generally are not considered to be neutron poisons (since by previous logic, they are part of the materials of construction). If subcriticality of the shipment is dependent upon the presence of these materials, the burden of proof that the materials will remain present during all normal and accidental

conditions is an evaluation issue (structural, containment, and watertightness), rather than an operational/quality assurance issue.

6.5 CALCULATIONAL METHOD

The calculational method used for the criticality analysis consists of the computer code(s) and cross-section set(s) used in evaluating the different configurations of interest. Other important elements of the analysis that govern how the code and cross-section data are employed should also be addressed in a manner that clearly conveys the steps taken in arriving at the results, including cross-section processing options (where applicable), special code options that may be invoked by the analyst, and criteria for calculational convergence. In the ensuing discussion, the use of "multigroup code" refers to a computer code such as KENO V.a,^[5] which is structured in a multigroup format, and requires some other calculational modules (BONAMI and NITAWL typically) to correct for resonance self-shielding and other effects and to convert raw cross-section data into a working library format. The term "continuous energy" will refer to a code such as MCNP^[6] or MONK^[7] that uses cross-section libraries that are essentially continuous in energy and do not need modules that adjust the basic cross-section data for resonance self-shielding, etc. Both categories of codes are available and are in use around the country.

6.5.1 Computer Codes

The computer codes and cross-section sets used in the evaluation should be uniquely identified and described in a level of detail commensurate with their familiarity in the packaging or criticality communities. Widely used codes (such as KENO V.a or MCNP) or code packages (such as SCALE^[8]) will probably require less description than a special use or unique computational method. All hardware and software (titles, versions, effective dates, etc.) used in performing the calculation should be identified.

Also to be included in this section are pertinent configuration control information and periodic validation test information.

6.5.2 Cross-Section Processing

This section discusses codes or modules that perform cross-section processing for resonance self-shielding, cell-weighting of mixtures, and other treatments en route to producing working library cross-section data. As was indicated earlier, these mathematical treatments are generally for multigroup codes and not for continuous energy codes. Using an example from the SCALE^[8] code package, the C5A525 sequence will automatically invoke BONAMI-S and NITAWL-S to provide resonance self-shielding corrected cross sections for the specified unit cell geometry (infinite homogeneous medium, lattice cell, or multiregion). In addition, in some sequences XSDRNPM-S can be used following BONAMI-S and NITAWL-S to flux-weight the cross-section set so that it describes the spatial variation of neutron flux within a unit cell configuration. Cross sections thus derived can be used in a homogeneous mixture to represent the neutronic behavior of a heterogeneous system.

Although cross-section processing using the standard SCALE geometries for the unit cell configuration may be adequate for many problems, there may be cases in which the unit cell arrangement is different from the standard geometries or in which it may be necessary to provide resonance-corrected cross sections for materials outside the unit cell. CSASN, which activates BONAMI-S and NITAWL-S, can be used to obtain Dancoff factors which are then input to KENO in the MORE DATA parameter field. Also, it is sometimes desirable to provide resonance-corrected cross sections for materials that appear in the lattice but are not included in the unit cell description. This can also be addressed by using the MORE DATA field. In any case, information should be provided that describes the procedures used

in arriving at working library format cross sections that are considered to best represent the neutronics of the problem.

In some instances using multigroup codes, the cross-section processing method used for one type of calculation should not be used for another type of calculation (for example, the method used for single units may not be technically correct for arrays of units). Correct processing of the cross sections into a working library depends on the analyst's ability to recognize patterns and/or changes in the neutron energies resulting from moderation and reflection. If the neutron energies are not correctly represented for cross-section processing, the resulting cross-section data in the working library will be incorrect. If one is calculating a uranium sphere (93% enriched in ^{235}U), the single unit calculations may employ the infinite homogeneous medium approximation depending on the size of the sphere. However, when an array of these spheres is calculated with moderation and reflection, a multiregion representation would better account for thermal neutrons that will be present near the surface of the sphere, and the cross sections should be processed accordingly. Many cross-section sets, both multigroup and continuous energy, have various scattering kernel data for elements such as hydrogen where scattering is very important. Whenever one of these special treatments is used, that fact should be pointed out and a technical explanation given as to why it is superior to the regular or other treatments.

6.5.3 Other Code Options

Most of the computer codes typically used for analyses provide varying means for describing reflectors, specifying starting distributions for neutrons, processing the cross-section data, and modeling infinite arrays. Whenever one of these techniques is used, it should be adequately identified in the analysis documentation.

6.5.4 Computational Convergence

Calculations made using Monte Carlo methods inherently contain uncertainties because of the statistical nature of the processes that are being simulated. Theoretically, as the number of particles tracked increases, the size of the standard deviation will decrease regardless of how close the result is to the "correct" answer. Identifying error (the deviation of the calculated result from the correct answer) is different from determining whether a calculation has adequately converged around "some" answer. Different random number sequences, various neutron starting distributions, and other methods can be used to investigate whether the answer given by a calculation is reproducible and therefore more likely to be near the "correct" answer. But the correct answer is almost always unknown, so one must look rather exclusively at calculational convergence as the criterion for sufficiency.

For most Monte Carlo codes, several pieces of information are given in the output which are useful when determining calculational convergence, including among others:

1. K-effective by generation run,
2. Plot of average k-effective by generation run,
3. Final k-effective edit table by generation shipped,
4. Plot of k-effective by generations skipped, and
5. Frequency distribution bar graph.

Conditions that may cause the questioning of convergence include the following:

1. Trends (upward or downward) in k_{eff} by generation run over the last half of generations run,
2. Trends in k_{eff} by generation for the first half of generations skipped,

3. Sudden changes of greater than one standard deviation in either y plot,
4. Abnormally high or low generation k_{eff} (+/- 20% of calculated mean), and
5. Calculated result that is not consistent with expectations.

Calculational convergence may be improved through various means such as running more histories, starting with an initial neutron distribution in the most reactive region of the model, or using biasing techniques. Note that grinding the standard deviation to a very small number using a large number of particle histories may produce an answer that appears to be of a higher quality than it actually is. Most calculational methods are accurate to only within a certain fraction of a percentage and this value may be higher than the percentage uncertainty derived from standard deviations presented with calculated answers. Typical standard deviation values for a properly converged calculation with 30,000 histories (an average number typically run) is between 0.003 and 0.006.

6.6 CALCULATIONAL RESULTS

This section emphasizes the calculations that should be performed, for the criticality evaluation, rather than interpreting the results of the calculations (which is the intent of this section in the actual SARP). The purpose of the criticality safety evaluation is to demonstrate the subcriticality of a single package and an array of packages, during NCT and during HAC, and to determine the transport index for criticality control purposes. The actual calculations necessary will be governed by the various parameter changes and conditions that must be considered and will be influenced by the packaging design and features, the contents, their susceptibility to damage, etc.

The calculated results should be presented as tables, and as a minimum should provide the case number, a brief description of the conditions, and the calculated results. Providing in the table additional

information that supports and/or simplifies the verbal description in the text may also be convenient. No specific format for the tables is required. The format used should be the one that most clearly presents the results and permits easy cross referencing between the table and the text. Tables 6.3 and 6.4 are provided as examples.

A TI must be determined for all fissile and radioactive material shipping packages. The TI is a dimensionless number that designates the degree of control to be exercised by the shipper or the carrier during transport. TI for purposes of radiation protection, (hereinafter called the RI) is the number expressing the maximum radiation level in millirems per hour at 1 meter from the external surface of the package. TI for purposes of criticality control for fissile material packages, (hereinafter called the CI), must be determined for both NCT and HAC. The higher of the NCT and HAC criticality indices becomes CI; the higher of the CI and RI becomes TI for purposes of package labeling. Any measured or calculated index greater than 0 must be rounded up to the first decimal place (therefore, an index measured or calculated to be 0.0001 is rounded up to 0.1).

The following discussion presents a logical, generic approach to the calculational effort. Two series of calculational cases should be performed: a series of single-unit cases and a series of array cases. Subsets of the array series for different size arrays may also be necessary. Each array series should include calculations for NCT (i.e., undamaged packages in an unmoderated array) and HAC (i.e., damaged packages in a moderated array).

Table 6.3. Example format of table for single-unit calculations

Single unit calculational results

Case	Water reflected ^a	Internal moderation ^b	AEG ^c	$k_{eff} \pm \sigma^d$
SU1	No	0.000		
SU2	Yes	0.000		
SU3	Yes	0.001		
SU4	Yes	0.003		
-	-	-		
-	-	-		
SUx	Yes	1.000		
SUy	No	1.000		

^a When reflected, water is ____ cm thick on all faces.

^b Internal moderation is the specific gravity of water in all void space inside the packaging; specific gravity is the ratio of actual water density of 0.9982 g/cm³.

^c Average energy group (AEG) is the average energy group causing fission.

^d σ is one standard deviation of the KENO calculated result.

Table 6.4. Example format of table for array calculations

Array calculational results

Case ^a	Array size	Internal moderation ^b	Interstitial moderation ^b	AEG ^c	$k_{eff} \pm \sigma^d$
IA1	Infinite	0.0	0.0		
IA2	Infinite	0.0	0.001		
IA3	Infinite	0.0	0.003		
-					
IAx	Infinite	0.0	1.0		
FA1	$7 \times 7 \times 7$				
FA2	$7 \times 7 \times 7$				
FA3	$7 \times 7 \times 7$				
-					
-					
FA10	$5 \times 5 \times 5$				
FA11	$5 \times 5 \times 5$				
-					
-					

^a Case identifier IA represents infinite arrays and FA represents finite arrays; all finite arrays reflect with ____ cm water.

^b Internal moderation is the specific gravity of water in all void space inside the packaging, and interstitial moderation is the specific gravity of water outside the packaging (between packages).

^c AEG is the average energy group causing fission.

^d σ is one standard deviation of the KENO calculated result.

6.6.1 Single-Unit Series

The single-unit (i.e., a single package) series of calculations are necessary because 10 CFR 71.55 requires that certain conditions be evaluated and are desirable as points of reference for subsequent calculations involving variations of certain parameters.

The single-unit series should start with a single, undamaged, as-shipped package. The remaining single-unit cases should systematically and progressively, reflect and flood the package to represent certain normal and accidental conditions. If HACs cause damage to the contents, the damaged configuration must also be considered. If a package has multiple containment boundaries, flooding each boundary consecutively should be considered. The final case of the single-unit series will represent a package completely flooded and reflected. Variations in the flooding sequence may be necessary, such as partial flooding, considering the package in the horizontal and vertical orientations, flooding (moderating) at less than full-density water, progressively flooding regions from the inside out, etc. The primary objective of the single-unit cases is to show that a single package is subcritical under normal and accidental conditions, under conditions specified by 10 CFR 71.55, and to identify the specific conditions that produce the highest neutron multiplication factor. Packaging designed for different fissile material loading configurations (including partial load configurations) will require a similar approach for each different loading, unless the contents model was developed to encompass the different loadings.

The systematic, progressive order to parametric variation of the single-unit cases, combined with the review of certain calculated nuclear characteristics (e.g., the neutron leakage fractions, the average neutron energy group causing fission, etc.) will greatly enhance the understanding of the neutron physics and interaction potential of the package to varying conditions. The results of the single-unit calculations can greatly influence the approach to and the number of calculations required for the array series

calculations. This is especially important if there are different content loading configurations. By thoroughly evaluating each different loading configuration and determining the most reactive conditions for each loading, it may be possible to minimize the number of array cases needed.

It must be understood that 10 CFR 71.55, "General Requirements for all Fissile Material Packages," has three different performance standards for the single package. Paragraph 71.55(b) requires (among other requirements, including liquid contents leaking out of the containment system) that water in-leakage into a single package to the most reactive credible configuration be considered, regardless of the watertightness of the containment boundary(s). Paragraph 71.55(d), for NCT, presumes that there will be no in-leakage into the containment system (unless it has been assumed that the packaging is not watertight and moderation is already present to cause maximum reactivity). Paragraph 71.55(e), for HAC, requires consideration of water moderation to be consistent with the damaged conditions. Therefore, packages with a containment boundary that remains watertight under normal and accidental conditions need not be evaluated with internal moderation from water leakage into the containment system for the array calculations. While undamaged and damaged conditions must be specifically addressed per 10 CFR 71.55(d) and (e), the requirements of 10 CFR 71.55(b) usually result in a higher k_{eff} for the single unit, unless the accident conditions alter the fissile material configuration. Consequently, the most reactive conditions from the single-unit calculations may not be the most appropriate for the array evaluations. Thus, an extensive investigation of the single-unit nuclear characteristics is necessary before starting the array calculations.

6.6.2 Array Series

Ideally, the first series of array calculations should be for an infinite array. If the infinite array is adequately subcritical under normal and accidental conditions, $CI = 0$, and no additional array

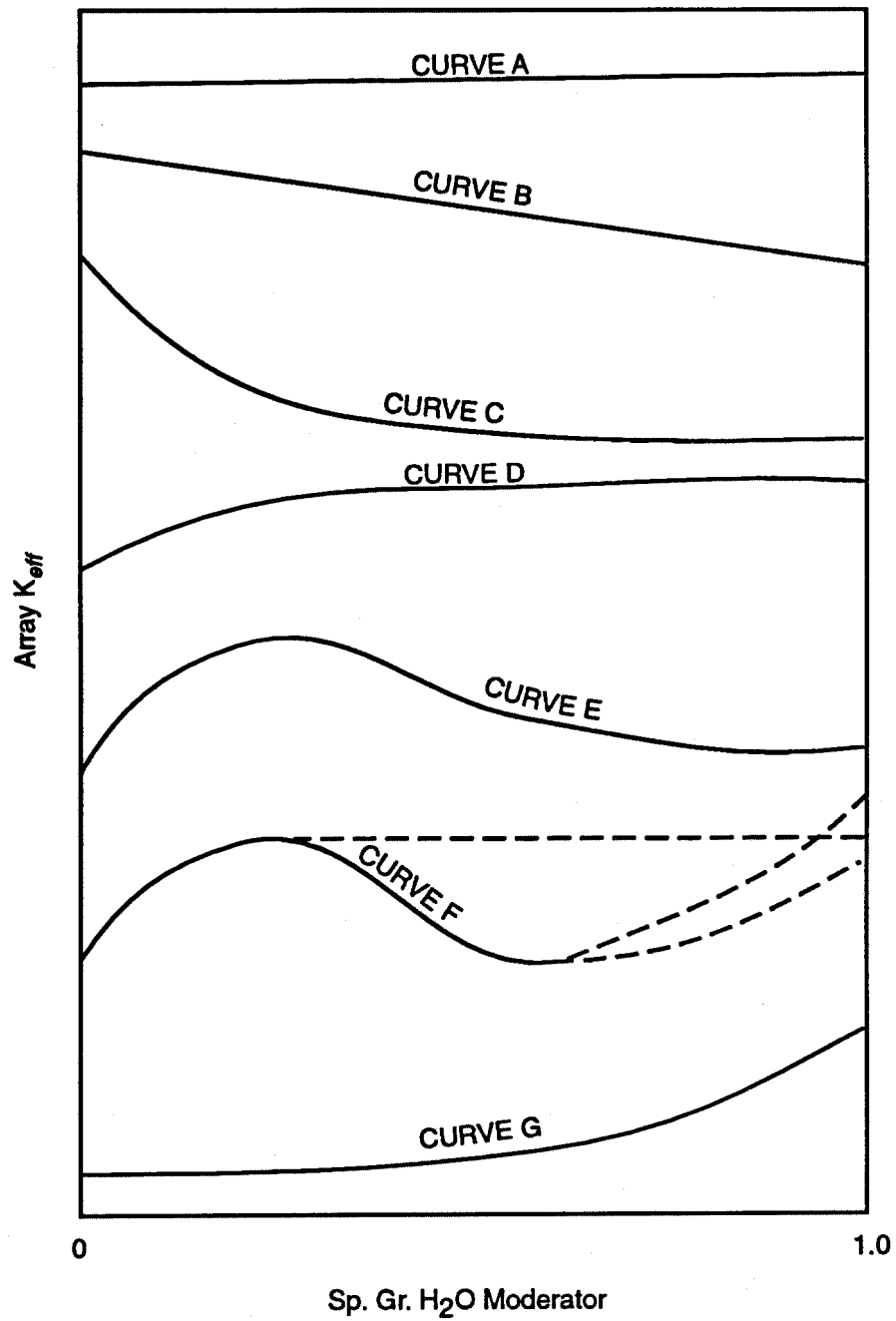
calculations are necessary. If either of the normal or accidental conditions are shown to be critical, or if the maximum k_{eff} exceeds the acceptable upper safety limit, a large finite array should be selected (e.g., a $12 \times 12 \times 12$ array) and all cases recalculated. Successively smaller finite arrays (e.g., $10 \times 10 \times 10$, $8 \times 8 \times 8$, $6 \times 6 \times 6$, etc.) may be required until the array sizes for normal and accidental conditions are found to be adequately subcritical. As an alternative, an applicant may start with any array size (for example, one that is based upon the number of packages planned to be shipped on a vehicle). If this number is significantly less than the maximum permissible (from the iterative process just described), CI will be unnecessarily high. While this approach is obviously conservative, the extra conservatism will penalize facilities which use the transport index as a means of limiting the size of package storage areas within the facility.

Each array series should start with the undamaged packages in an unmoderated array. Varying amounts of interstitial hydrogenous moderation should be added in all floodable regions within and between the packages by varying the density of water in these regions. The water density should be varied from zero (unmoderated) to full density (flooded) in increments such that the optimum moderating density is determined, if an optimum actually exists. Usually, eight to ten calculations will be sufficient to determine the optimum. By graphically representing the multiplication factor, k_{eff} as a function of the moderator density, the response or trend of the plot may be determined. If k_{eff} remains constant or continuously decreases as moderator density increases, no optimum exists, and maximum reactivity occurs when it is unmoderated. If k_{eff} increases as moderator density increases and then begins to decrease (or remains constant at a plateau) as moderator density continues to increase, the conditions of optimum moderation occur at the maximum k_{eff} . However, if k_{eff} continuously increases as the moderator density increases and does not peak or reach a plateau before full-density moderator has been achieved, the optimum moderating conditions may not have been achieved.

For unmoderated infinite array calculations, the spacing of the packages is unimportant and does not affect k_{eff} . However, as an interstitial moderator is added to the region between packages, the spacing may become very important because of the amount of moderator that may be present. For this reason, it is usually advisable to place a tight-fitting cuboid boundary around the array calculational model. Specular and periodic boundary conditions on the cuboid will then duplicate a square-pitch infinite array of packages in contact in all three directions. If the k_{eff} response to increasing moderator density does not peak or achieve a plateau before full-density moderation is achieved, it will be necessary to increase the size of the cuboid surrounding the array model and to recalculate. Increasing the size of the cuboid provides an edge-to-edge spacing between packages, making more volume available for the moderator. To emphasize this situation, consider a cylindrical shipping package with a diameter of one unit and a height (or length) of two units. With a tight-fitting cuboid around the cylinder, 21.5% of the cuboid's volume is outside the package and is available for a moderator.

By increasing the cuboid's dimensions such that the edge-to-edge spacing between the packages in all directions is 10% of the package diameter, 38.2% of the cuboid's volume is outside the package and is available for moderator. This small increase in edge-to-edge spacing corresponds to a 126.0% increase in volume available for the moderator. Therefore, if maximum or optimum k_{eff} has not been achieved with the packages in contact, increasing the packaging spacing to permit additional moderation will be necessary.

Figure 6.5 depicts some typical array k_{eff} versus moderator density plots that may be encountered in shipping package criticality safety evaluations. Curves A, B, and C represent arrays for which an optimum moderator density does not exist; the maximum k_{eff} occurs with no moderator. Curves D, E, and F represent arrays for which an optimum moderator density does exist. The maximum k_{eff} occurs at the optimum; the optimum moderator density for curve D occurs over a range of values (i.e., the



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Fig. 6.5. Typical plots of array k_{eff} vs. specific gravity water moderation.

plateau), and for curves E and F a distinct peak is present when an optimum "peak" occurs as a result of interstitial moderator. The optimum moderator density may be very low (e.g., from 0.001 to 0.1). Therefore, when selecting the values of interstitial moderator density to calculate in the search for optimum, one should investigate this very low-density region.

Curve F is unusual in that an optimum moderator density has been achieved; as the moderator density is increased beyond the optimum, k_{eff} decreases because of the isolation properties of the moderator but then begins to increase because of the reflection of individual units. The array k_{eff} increase (after the minimum) may or may not exceed the k_{eff} at optimum moderation; however, it cannot exceed the k_{eff} of a corresponding flooded, fully reflected, single unit. If the array k_{eff} at full-density moderator is less than the k_{eff} of the flooded and reflected single unit, the edge-to-edge spacing of the packages is insufficient to permit full reflection. However, for curve F-type responses, there is no need to increase spacing and recalculate because the maximum k_{eff} of the array will be that of the reflected single unit or the k_{eff} of the optimum moderator density, whichever is larger. For curves A through F, the array k_{eff} at full-density moderation typically will be the same (within statistical limits) as the flooded and reflected single-unit case.

Curve G represents an array for which the optimum moderator density has not been achieved and the maximum k_{eff} has not been determined. For this situation, the center-to-center spacing of the packages in the array must be increased and all cases recalculated. The center-to-center spacing must be sufficiently large for the curve either to reach a plateau (like curve D) or to peak and then decrease (like curve E).

6.6.3 Interstitial Moderation

In the preceding section, array moderation was discussed as a parameter but only generally. In a package criticality evaluation, numerous conditions exist for which the effects of moderation must be investigated, such as 1) moderation from hydrogenous packing materials, which are usually inside the primary containment boundary; 2) moderation from hydrogenous materials of construction, e.g., thermal insulation and neutron shielding; and 3) the region between the packages in an array external to the package. The treatment of array moderation can be very easy or very complex, depending upon the type of placement of the materials of construction and their susceptibility to damage from hypothetical accident testing.

For determining CI of a package for NCT, only the hydrogenous moderator present in the package need be considered [items 1) and 2) above]; moderation between packages [item 3) above] from rain, snow, flooding, etc., is not required per 10 CFR 71.59(a)(1). Determining CI of a package for HAC must consider all three conditions, including how each form of moderation can change. For example, for a spent fuel shipping cask with no hydrogenous thermal insulation or neutron shielding materials, no internal moderation is present for the NCT and only water moderation between packages (mist, rain, snow, and flooding) for the HAC. However, for a package with thermally degradable insulation, the analyst will need to evaluate both arrays with the undamaged insulation and no additional moderation for NCT and evaluate the effects of reduced moderation from the thermal tests as well as increased moderation from water submission tests, with water moderation between the packages, for HAC. If the inner containment vessel is not a high-integrity, water-tight container, varying degrees of moderation in that region must also be evaluated. For all such conditions and combinations of conditions, the optimum degree of moderation must be found and shown to be adequately subcritical.

6.6.4 Determining the Criticality Index

The array series must evaluate arrays of undamaged, unmoderated packages (NCT) and damaged, optimally moderated packages (HAC). From these results, CI is determined. Per 10 CFR 71.59(a)(1), five times "N" undamaged packages with nothing between the packages must be subcritical, and, per 10 CFR 71.59(a)(2), two times "N" damaged packages would be subcritical with optimum interspersed hydrogenous moderation. Per 10 CFR 71.59(a), each array of packages must be water reflected (except infinite arrays). CI is determined by dividing the number 50 by the values of "N" for each of the two conditions, and the higher of the two indices becomes the CI. In equation notation,

$$CI_{NCT} = \frac{50}{N_U} = \frac{50}{1/5 X_U} = \frac{250}{X_U}$$

$$CI_{HAC} = \frac{50}{N_D} = \frac{50}{1/2 X_D} = \frac{100}{X_D}$$

where

N_U = the number of packages that may be shipped based upon NCT criteria;

N_D = the number of packages that may be shipped based upon HAC criteria;

X_U and X_D = the maximum number of packages determined to be subcritical for undamaged conditions (U) and damaged conditions (D), respectively;

$$N_U = 1/5 X_U ,$$

$$N_D = 1/2 X_D .$$

The higher of these two CI values becomes CI for the package; the higher of CI and RI becomes TI for package labeling. Per 10 CFR 71.59(b), any CI greater than zero must be rounded up to the first decimal place. Therefore, for a fissile material package to have a $CI = 0$, an infinite array must be subcritical for both NCT and HAC.

6.7 CALCULATIONAL METHOD VALIDATION

The validity of the calculational method (computer code and material nuclear properties cross-section data sets or libraries) used for the evaluation of nuclear criticality safety must be established and documented. In support of the safe transportation of fissile material, the calculational method validation documentation may be included in SARP, or it may be published as a separate report with important features summarized in the appropriate SARP section. This section of the guide discusses important features and summary descriptions. Although there are many different approaches to validating a calculational method, the general procedure included in this section of the guide should be common to all approaches. The validation effort will consist of selecting benchmark critical experiments (or possibly certain subcritical experiments that meet some stringent requirements), calculating the effective neutron multiplication factors of the experiments using the chosen computer code/cross-sections library combination, establishing the calculational bias and uncertainties, establishing the area of applicability, and then determining an acceptance criteria that ensures subcriticality for future calculations of unknown systems. The acceptance criteria must include not only the bias and uncertainty in the bias but also some additional margin of subcriticality.

Criticality safety computer code validations tend to be one of two types, specific or global. The specific validation models "a few" critical experiments that are very similar to the problem being evaluated. This type of validation is performed to satisfy the validation requirements of a code for a

specific application and has a limited area of applicability. The global validation models many critical experiments covering a wide range of conditions. This type of validation is performed to satisfy the validation requirements of a code for general applications and has a wide area of applicability. Although the effort required to perform a global validation may be significantly more than the effort to perform a specific validation, each method has the following four basic, identical goals: 1) to determine the calculational bias, 2) to determine the uncertainty of the bias, 3) to determine the range (or area) of applicability, and 4) to establish acceptance criteria for subcriticality.

6.7.1 Benchmark Critical Experiments

A very important aspect of the computer code method validation process is the quality of the benchmark critical experiments used. For nuclear criticality safety applications, the ability of the highly complex series of computer code steps and the associated nuclear properties of materials to predict/calculate accurately the reactivity of a series of well-characterized, documented experiments provides the basis upon which the credibility of the code/library combination is judged. This comparison of calculated results with known measurement results provides the data for development of the bias, the uncertainty of the bias, and the acceptance criteria.

In the past, it was customary in the past to use only critical experiments for the validation process, as these experiments presumably have an effective neutron multiplication factor of 1.0000. However, many of the “critical” experiment results included in reports and documents over the years are not true critical experiments, but actually contain extrapolations from subcritical conditions to critical for one or more physical or nuclear parameters. For example, a reported critical mass may actually be an extrapolation from a subcritical mass, extrapolated to critical by means of buckling conversion. This fact may not be obvious from the experiment report, but it may be discussed and justified in the original

experiment documentation. This kind of adjustment to the original either data may not be significant or it could be enough to invalidate the experiment for the intended use as a "benchmark critical experiment." Also, new subcritical measurement techniques are being developed that may result in substantially subcritical experiments being usable for computer code validation activities.

For nuclear criticality safety evaluations for the safe transportation of fissile materials, the critical experiments used as benchmarks for code validation should be similar to and representative of the packaging and contents being evaluated. For example, a series of critical experiments involving plutonium metal would not be appropriate for shipments of uranium metal. The benchmarks' physical compositions, geometric configurations, and other nuclear characteristics should be reviewed to ensure applicability (similarity) to both current and future problems (contents and packaging materials) that the validation is intended to cover. Unfortunately, critical experiments available for use as benchmarks tend to emulate only the contents of a single package under hypothetical accident conditions (i.e., water flooding). However, a package evaluation for certification will require calculations of four conditions: single package-normal conditions, hypothetical accident conditions, arrays of packages-normal conditions, and hypothetical accident conditions. Finding sufficient critical experiments or other "benchmark" experiments to provide the area of applicability needed for a particular transportation application may be difficult if not impossible. Therefore, including a wide variety of benchmark experiments in the validation work maybe necessary to adequately assess the validity of the calculational method used in the application evaluation.

6.7.2 Calculational Bias

For nuclear criticality safety applications, the calculational bias associated with a calculational method validation can be defined as a measure of the systematic disagreement between the results

calculated by a method (the computer code and its associated cross-section library) and experimental data. The usual method of determining the calculational bias is to correlate the results of the benchmark critical experiments with the calculated results of the method being validated. With a value of unity (i.e., $k_{\text{eff}} = 1.0000$) for each benchmark critical experiment, the bias is the deviation of the calculated values of k_{eff} from unity.

The average bias is usually determined by one of two methods: 1) taking the difference between a simple average of the calculated results and unity, which may be adequate for a specific validation, or 2) taking the difference between a linear regression of the calculated results (as a function of some independent variable) and unity, which is usually necessary for a global validation. The first method produces a single value for the bias, whereas the second method produces a variable bias that is a function of the independent variable. This bias varies because of trends that may change over the range of the independent variable. Generally, neither the bias nor its uncertainty is constant; both should be expected to be a function of one or more nuclear or physical variables, especially if there is to be a wide area of applicability. Physical variables include such parameters as material composition, density, enrichment, etc., and nuclear variables include the average energy group (AEG) of the neutrons causing fission, the ratio of thermal absorptions to total absorptions, the ratio of total fissions to thermal fissions, etc.

6.7.3 Uncertainties

Uncertainties in the calculational results in a validation come from three general sources. The first source is from the original critical experiment and the experimenter(s), which may include uncertainties in the material composition and fabrication tolerances of the equipment hardware (experimental apparatus) and fuel materials (compositions, assays, masses, densities, dimensions, etc.),

from the experimenters' manipulation of and/or adjustments to the experimental data from an inadequate (including inaccurate or incomplete) description of the experimental layout and surroundings, etc. The second source is from the computational technique itself, which may include uncertainties in the mathematical equations solved in the computer code, calculational approximations used in solving the mathematical equations, the computer code convergence criteria, the cross-section data and the manipulation of the cross-section data, limitations of the computer hardware, etc. The third source is from the analyst and the calculational models developed to simulate the experiment, which may include uncertainties because of material composition and dimensional modeling approximations, the selection of various code options, individual modeling/coding techniques, interpretation of the calculated results, etc.

The preceding discussion is not intended to identify and define all sources of uncertainty but to alert those performing calculational method validations (code validators) that there are many potential sources of uncertainties. Of these three sources of uncertainties, code validators usually have no control over the first and second sources and very little control over the third source. However, for code validation purposes, it is usually neither practical nor necessary to quantify and qualify all the individual uncertainties. In practice, the code validator can estimate the total uncertainty through application of a valid statistical treatment of the calculational results of the benchmark experiments. The total uncertainty determined usually appears as the bias and a variability in the bias, depending upon the statistical analysis applied. The combination of the bias and the uncertainty in the bias is deduced from the (statistical) mean k_{eff} to establish a minimum k_{eff} value. This minimum value (and any larger k_{eff} values) is then considered to be critical with the confidence limits applied to the statistical technique to determine the uncertainty. Another way of looking at this is that a future calculational result, performed within the limitations of the validation method (computer code, cross sections, modeling, etc.) will be considered to be subcritical if the calculational result plus its corresponding calculational uncertainty (usually two standard deviations

for Monte Carlo methods) is less than the minimum k_{eff} value; any result equal to or greater than the minimum k_{eff} value but below 1.0000 is considered critical (cannot be considered to be subcritical).

One as yet unmentioned additional source of uncertainties cannot be addressed during the initial calculational method validation. One must take into account the uncertainties in dimensional and material tolerances and specifications of future problems to be calculated must be taken into account. This statement refers to all of the calculational models developed for use with the "validated code package" other than the "benchmark critical experiments" used in the validation. Because it is impossible for the code validator to predetermine uncertainties that may be encountered in future problems, the code user (i.e., the criticality analyst) must eliminate this source of uncertainty during the development of the calculational models for the future problems. Following the guidance provided in Sect. 6.3, "Calculational Models (Dimensional)," and Sect. 6.4, "Model Materials (Densities)," conservative calculational models will be developed such that any dimensional and material specifications and tolerances need not be a concern. Potential uncertainties resulting from the 10 CER 71 hypothetical accident testing (e.g., amount of deformation and loss of spacing from drop tests, effects on materials from thermal tests, etc.) can also be addressed in the development of the calculational models.

6.7.4 Area of Applicability

An integral part of a code validation effort is to define the area and range of applicability for which the validation is applicable. The area of applicability is intended to describe generically the type of system by identifying the important parameters and/or characteristics for which the calculational method was (or was not) validated. For example, the area of applicability may need to include specific types of fissile materials [highly enriched uranium (HEU), low-enriched uranium (LEU), plutonium (Pu) of low ^{240}Pu content, etc.], material compositions (solution or metal, water-moderated or carbon-

moderated, etc.), geometric configurations (single units or arrays, heterogeneous or homogeneous, etc.), reflector materials (water, steel, etc.), etc. The range of applicability is intended to identify specific limits (upper and lower) of the parameter or characteristic used to correlate the bias and uncertainties. For example, the range of applicability may be defined in terms of the moderating ratio (e.g., $H/X = 10$ to 500), in terms of the average energy group of the neutrons causing fission (e.g., $AEg = 6.5$ to 21.5), or in terms of the ratio of total fissions to thermal fissions (e.g., $F/F_{th} = 1.0$ to 5.0). For subsequent use of a validated code, the analyst should justify that the parameters and characteristics of the problem being calculated fall within the area and range of applicability defined during the calculational method validation.

6.7.5 Acceptance Criteria

Determination of the bias and uncertainties establishes a minimum k_{eff} value for which a system with a higher calculated k_{eff} is considered to be critical within the confidence limits applied during the statistical evaluation of the benchmark calculated data. A margin of subcriticality, usually in terms of k_{eff} , must be deduced from the minimum k_{eff} value described earlier to ensure subcriticality when the criticality safety of a system is based upon k_{eff} calculations.

Numerous ANSI/ANS standards^{[9],[10],[11],[12],and[13]} and an NRC regulatory guide^[14] address code validation requirements and the establishment of a margin of subcriticality (ANSI/ANS-8. 17^[10] is the only reference that specifically mentions transportation). Basically, Refs. 8 through 14 use the following relationship (with some variations in definitions and subscript notation):

$$k_a < k_c - \Delta k_u - \Delta k_m,$$

where

k_a is the maximum allowable calculated k_{eff} ,

k_c is the mean k_{eff} resulting from the calculations of the benchmark experiments (may include biases and uncertainties not included in Δk_u),

Δk_u is an allowance for uncertainties in the experiments and calculational technique (if not accounted for in k_c),

Δk_m is the required margin of subcriticality.

All the cited references state that a margin of subcriticality, Δk_m , should be provided. References 11, 12, and 13 state that a Δk_m of 0.05 should be assumed unless a smaller value can be justified, but in no case should a value of less than 0.02 be used; Refs. 8, 9, and 14 do not recommend specific values for Δk_m .

A common practice has been to arbitrarily assume a maximum allowable k_{eff} , usually a value of 0.95, without regard to biases, uncertainties, or a margin of subcriticality. Any calculated k_{eff} plus (typically) two standard deviations that is less than 0.95 would be acceptably subcritical with this method. Without the benefit of a validation study to estimate the biases and uncertainties, the use of a preset maximum value may not be adequately subcritical, or it may be unnecessarily conservative.

The acceptance criteria should be based upon a statistically valid technique that provides allowances for the bias and uncertainty over the range of applicability. A margin of subcriticality must be provided in accordance with national standards or guidelines.

6.8 QUALITY ASSURANCE

Quality Assurance activities for all related packaging activities including criticality aspects must conform with the applicable requirements of DOE Order 5700.6C, 10 CFR 71, Subpart H, or other relevant codes and standards.

The selective application of Quality Assurance requirements begins with the adherence with engineering procedures for the control of all activities during the design of the packaging. These approved procedures typically include control of design input, data and assumptions, document control, change control, design verification, control of software, and interface controls.

A nonconformance and corrective action system should be in place to handle deviations or non-conformances identified during the design process. Deviations to requirements and procedural controls should be documented and appropriate personnel identified to evaluate adequately and to disposition each deviation.

A record-keeping system should be established and records of the design must be maintained according to approved procedures.

Periodic internal assessments of the adequacy of the design control systems should be accomplished by the Engineering organization to ensure the effectiveness of these controls.

The principle quality assurance activities related to the criticality safety evaluation can be divided into three major categories: development of the calculational models, the computational technique, and the computer code software/hardware.

Development of the computational model (described in Sects. 6.3 and 6.4) contains many elements for which quality assurance must be addressed, such as the following: 1) the adequacy of the models to dimensionally represent the packaging and contents, 2) the adequacy of the models to materially represent the packaging and contents, 3) the changes in the dimensions and materials representing the packaging and contents for varying conditions (undamaged and damaged packages and normal conditions and accident conditions), 4) the reference sources of the dimensions and of the material densities, compositions, etc., used in the various calculational models, and 5) configuration control between the package design and the calculational models.

The computational technique (described in Sects. 6.5 and 6.6) contains many elements for which quality assurance must be addressed, such as the following: 1) converting the calculational model (dimensions and materials) into an input format for the computer code, 2) using the code within defined limitations and restrictions, 3) interpretation of the code output, 4) application of the calculated results, and 5) documentation of the results.

Code software/hardware (described in Sect. 6.7) also contains many elements for which quality assurance must be addressed, such as the following: 1) validation of the computer code to benchmark experiments, 2) determining the bias and uncertainty of the code, 3) establishing a margin of subcriticality or other defined safety margin, 4) determining the range of applicability of the code, and 5) the software/hardware configuration control plan.

6.9 REFERENCES

1. U.S. Department of Transportation, *Packaging and Transportation of Radioactive Material*, Code of Federal Regulations, Title 10, Part 71, Washington, D.C., January 1993.
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